

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
 Data File : BG050516.D
 Acq On : 8 Oct 2021 19:39
 Operator : CG/JU
 Sample : M4117-17
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-5(3.0-3.5)

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050516.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.329	306	313	319	rBV	35758	57461	2.29%	0.376%
2	5.799	385	393	402	rBV	781396	1287081	51.38%	8.416%
3	7.398	657	665	678	rBV	805226	1442053	57.56%	9.430%
4	8.261	803	812	819	rBV	175464	312124	12.46%	2.041%
5	9.430	1003	1011	1020	rBV	513741	939955	37.52%	6.146%
6	10.829	1241	1249	1257	rBV	145809	247462	9.88%	1.618%
7	11.081	1285	1292	1300	rVB	240505	443612	17.71%	2.901%
8	13.502	1696	1704	1713	rVB	1210738	1892909	75.56%	12.378%
9	14.877	1929	1938	1945	rBV	388997	616717	24.62%	4.033%
10	16.358	2183	2190	2202	rVB	853792	1306770	52.16%	8.545%
11	17.621	2398	2405	2409	rBV	458473	727667	29.05%	4.758%
12	17.662	2409	2412	2419	rVB	51677	78224	3.12%	0.512%
13	18.255	2508	2513	2517	rBV2	34080	47419	1.89%	0.310%
14	18.479	2546	2551	2557	rBV4	34571	77133	3.08%	0.504%
15	18.537	2557	2561	2567	rVB2	30957	46807	1.87%	0.306%
16	18.678	2580	2585	2590	rBV4	27506	56661	2.26%	0.371%
17	18.720	2590	2592	2597	rVB2	23286	26999	1.08%	0.177%
18	19.389	2701	2706	2708	rBV	36545	55061	2.20%	0.360%
19	19.413	2708	2710	2715	rVB3	32481	41075	1.64%	0.269%
20	19.536	2726	2731	2739	rBV4	21168	41946	1.67%	0.274%
21	19.660	2747	2752	2757	rVB	159505	236535	9.44%	1.547%
22	20.018	2808	2813	2820	rVB	183134	278717	11.13%	1.823%
23	20.112	2820	2829	2835	rBV	165290	243573	9.72%	1.593%
24	20.206	2839	2845	2851	rBV	1869244	2505180	100.00%	16.382%
25	20.347	2863	2869	2875	rVB6	21075	51604	2.06%	0.337%
26	20.664	2919	2923	2928	rVB3	37649	49062	1.96%	0.321%
27	20.805	2943	2947	2952	rBV2	29931	42083	1.68%	0.275%
28	20.852	2952	2955	2963	rVB2	24177	42150	1.68%	0.276%
29	21.070	2988	2992	2999	rBV4	31564	55557	2.22%	0.363%
30	21.281	3024	3028	3034	rVB2	32386	54041	2.16%	0.353%
31	21.516	3064	3068	3074	rVB3	100396	143930	5.75%	0.941%
32	21.916	3128	3136	3142	rBV2	415137	886889	35.40%	5.799%
33	21.969	3142	3145	3152	rVB	90720	144596	5.77%	0.946%
34	24.237	3526	3531	3539	rBV3	40710	124073	4.95%	0.811%
35	25.329	3709	3717	3727	rVB3	234552	689580	27.53%	4.509%

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SB-5(3.0-3.5)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

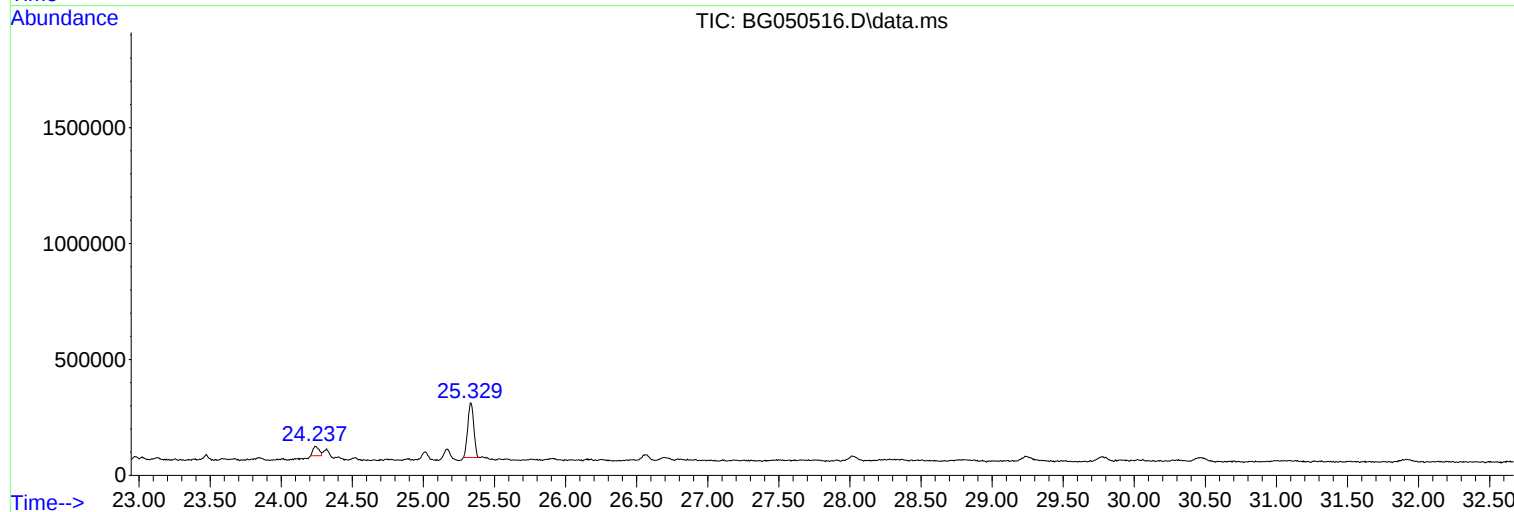
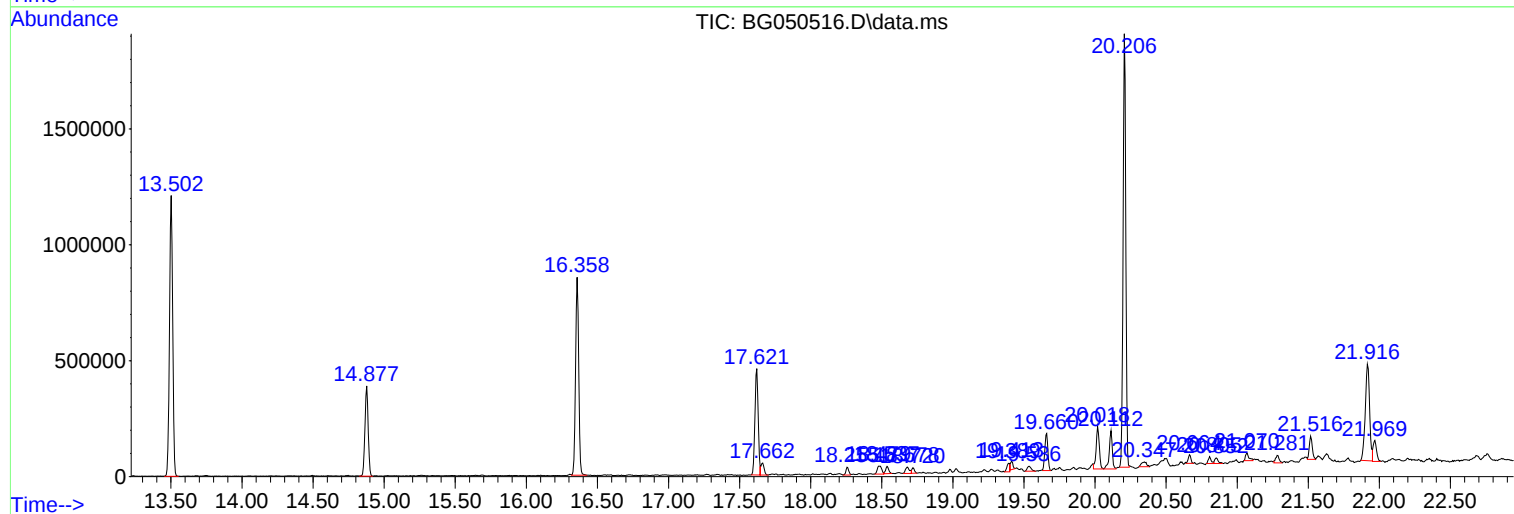
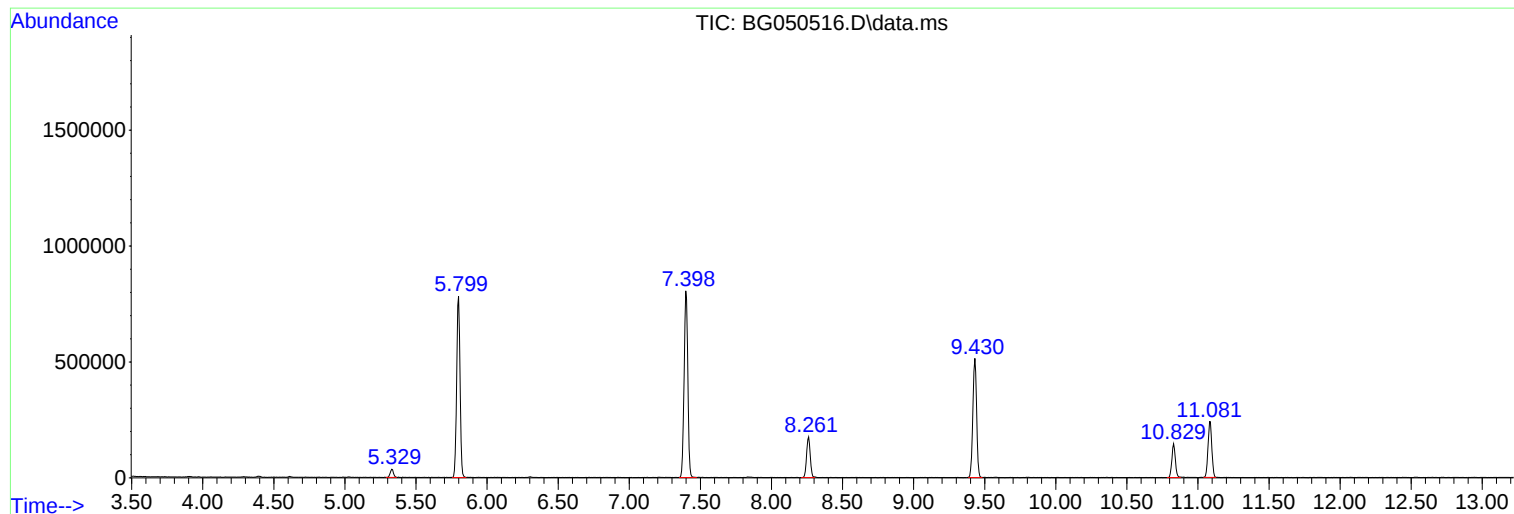
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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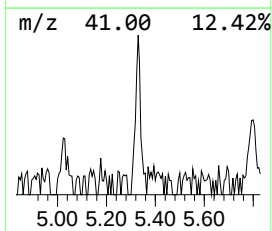
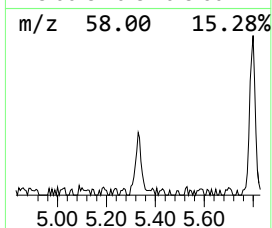
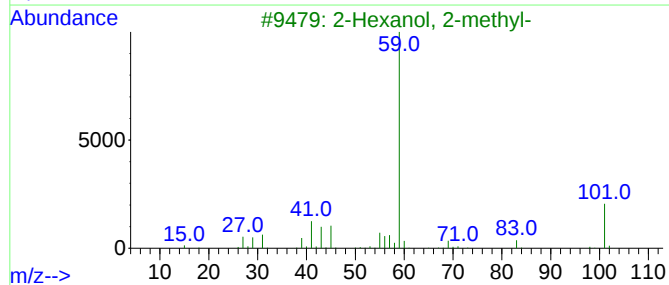
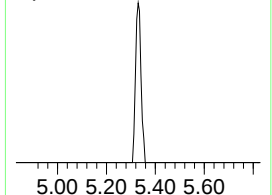
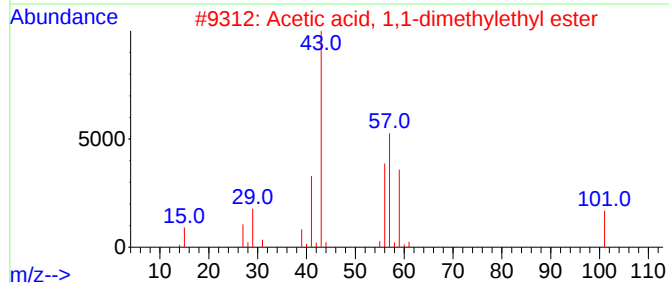
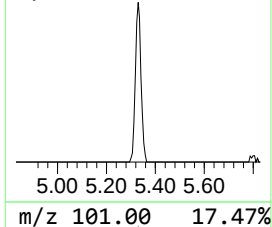
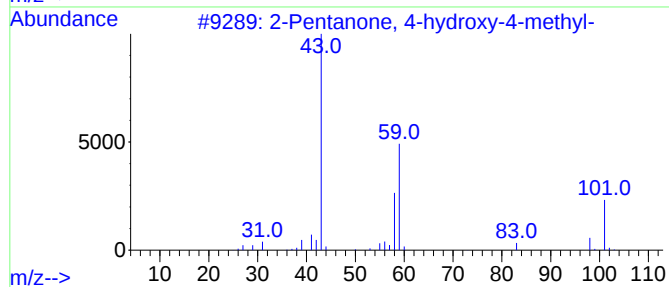
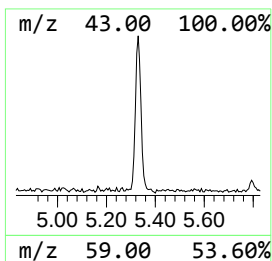
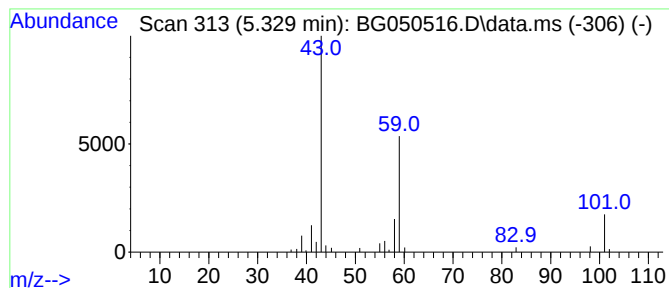
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.329	3.68 ng	57461	1,4-Dichlorobenzene-d4			8.261

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23	
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23	



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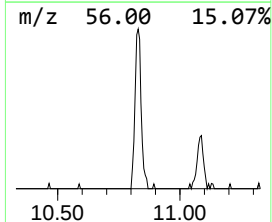
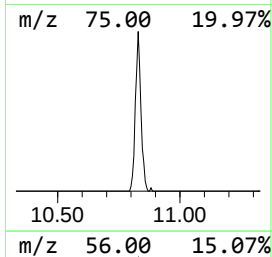
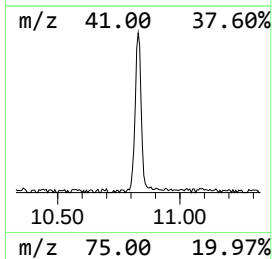
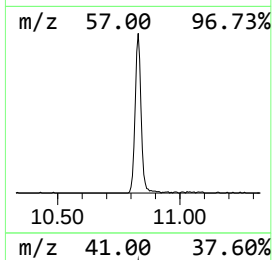
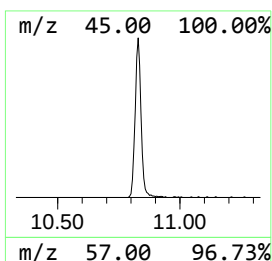
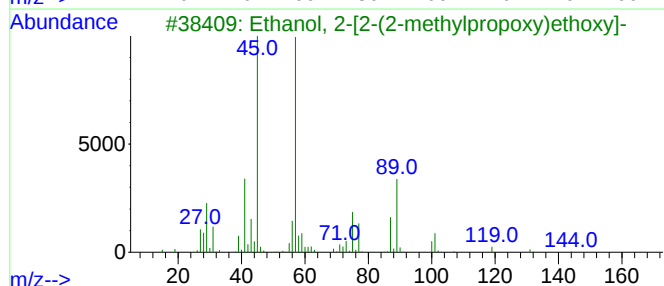
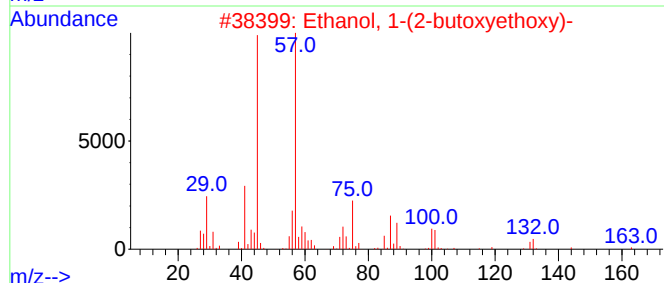
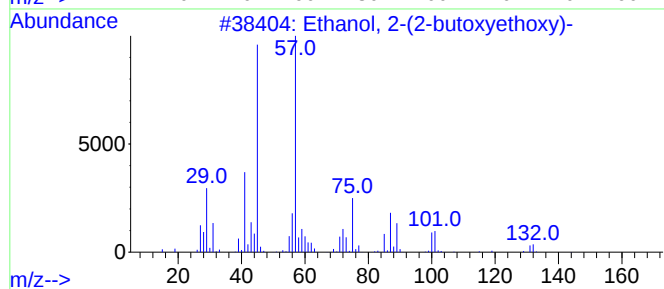
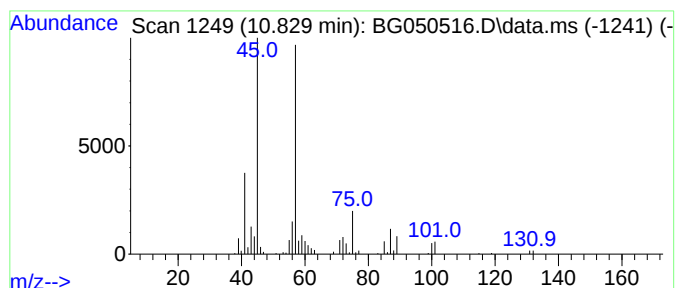
Instrument :
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SB-5(3.0-3.5)

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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.829	11.16 ng	247462	Naphthalene-d8	11.082	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50



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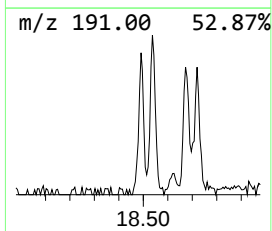
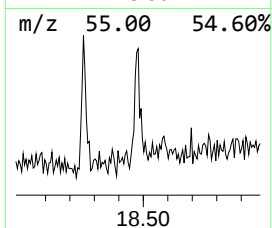
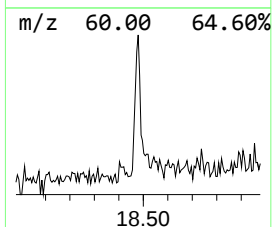
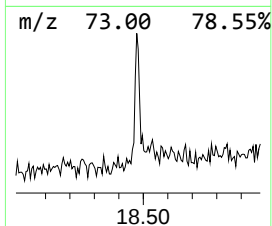
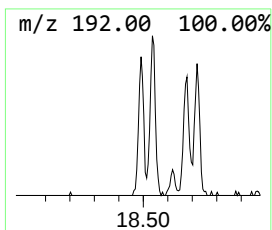
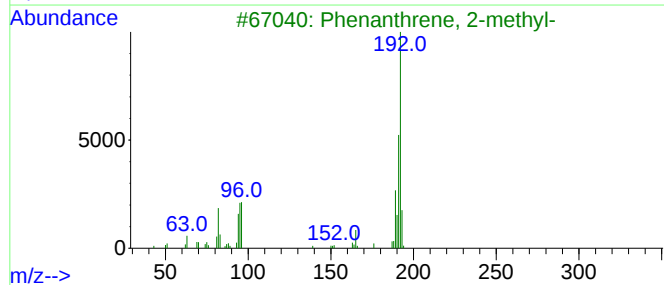
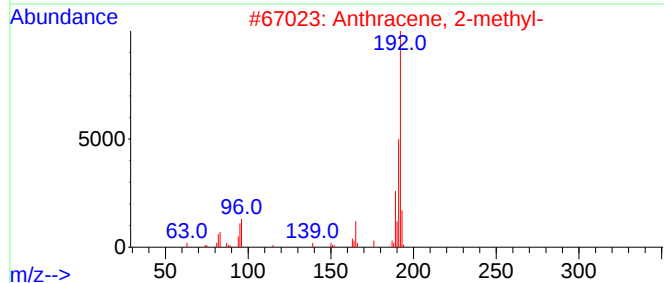
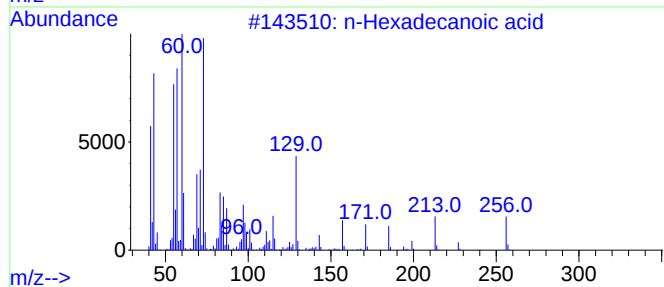
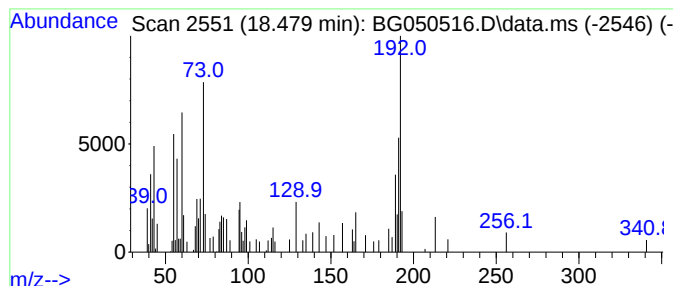
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.479	2.12 ng	77133	Phenanthrene-d10	17.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	60
3			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	55
4			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	55
5			Anthracene, 9-methyl-	192	C15H12	000779-02-2	55



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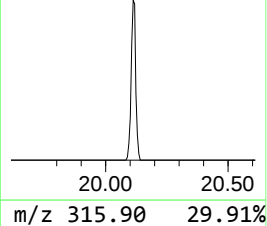
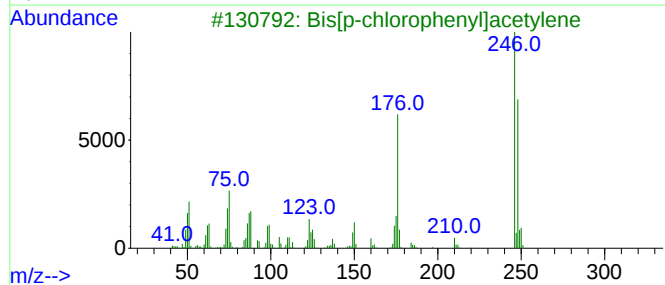
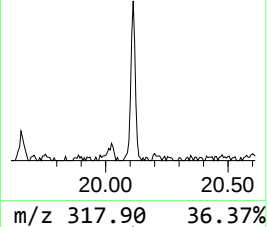
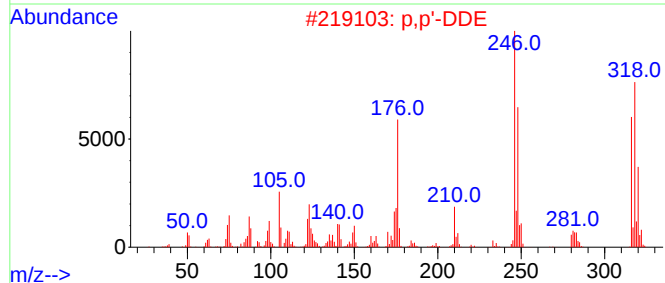
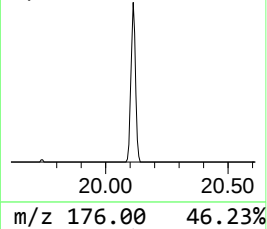
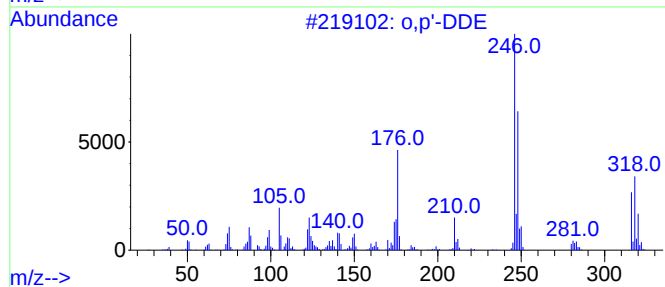
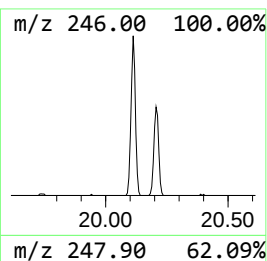
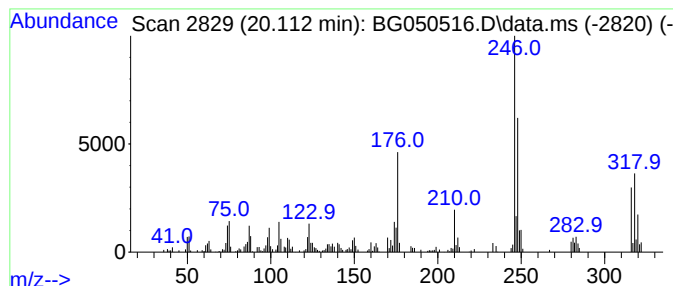
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 o,p'-DDE Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.112	5.49 ng	243573	Chrysene-d12	21.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o,p'-DDE	316	C14H8Cl4	003424-82-6	99
2			p,p'-DDE	316	C14H8Cl4	000072-55-9	99
3			Bis[p-chlorophenyl]acetylene	246	C14H8Cl2	001820-42-4	95
4			Anthracene, 9,10-dichloro-	246	C14H8Cl2	000605-48-1	94
5			9H-Fluorene, 9-(dichloromethylene)-	246	C14H8Cl2	000835-17-6	93



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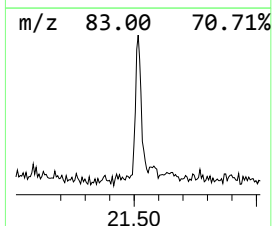
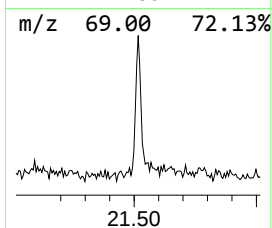
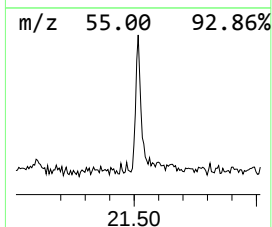
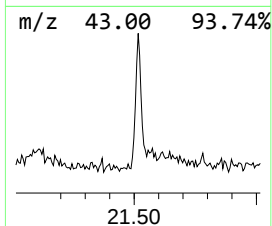
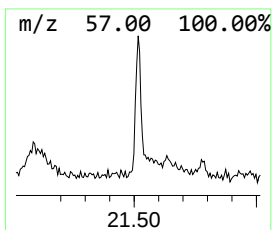
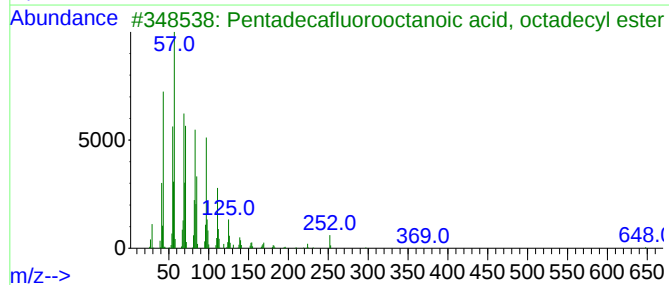
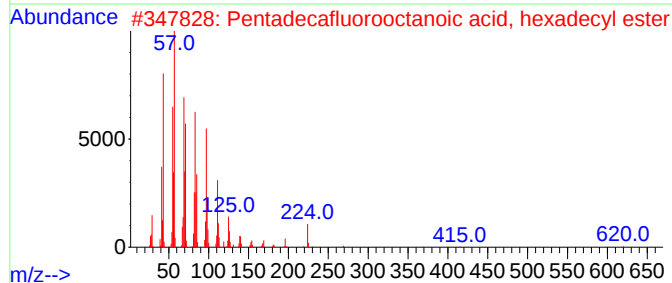
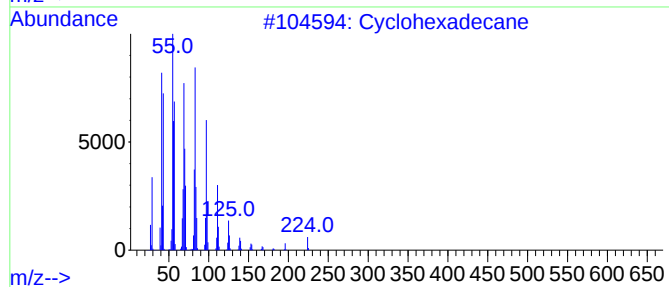
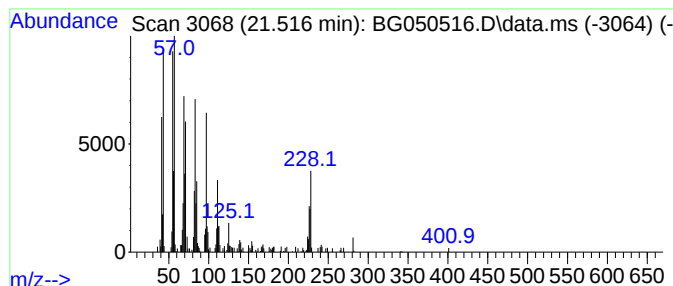
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.516	3.25 ng	143930	Chrysene-d12	21.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	93
2			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	89
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	89
4			1-Nonadecene	266	C19H38	018435-45-5	87
5			Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
Data File : BG050516.D
Acq On : 8 Oct 2021 19:39
Operator : CG/JU
Sample : M4117-17
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-5(3.0-3.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.329	3.7	ng	57461	1	8.261	312124	20.0
Ethanol, 2-(2-b...	10.829	11.2	ng	247462	2	11.082	443612	20.0
n-Hexadecanoic ...	18.479	2.1	ng	77133	4	17.621	727667	20.0
o,p'-DDE	20.112	5.5	ng	243573	5	21.916	886889	20.0
Cyclohexadecane	21.516	3.3	ng	143930	5	21.916	886889	20.0